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Kinetic Plasma Modeling with Quiet Monte Carlo Direct Simulation

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Abstract. The modeling of collisions among particles in space plasma media poses a challenge for computer simulation. Traditional plasma methods are able to model well the extremes of highly collisional plasmas (MHD and Hall-MHD simulations) and collisionless plasmas (particle-in-cell simulations). However, neither is capable of treating the intermediate, semi-collisional regime. The authors have invented a new approach to particle simulation called Quiet Monte Carlo Direct Simulation (QMCDS) that can, in principle, treat plasmas with arbitrary and arbitrarily varying collisionality. The QMCDS method will be described, and applications of the QMCDS method as "proof of principle" to diffusion, hydrodynamics, and radiation transport will be presented. Of particular interest to the space plasma simulation community is the application of QMCDS to kinetic plasma modeling. A method for QMCDS simulation of kinetic plasmas will be outlined, and preliminary results of simulations in the limit of weak pitch-angle scattering will be presented.

1 Introduction

Many space plasma media are semi-collisional, meaning that the collision times are comparable to the dynamical time scales of interest in the systems. In such plasmas the collisionality often varies considerably as a function of time or position. These systems include, for example, Earth's ionosphere, the solar chromosphere and corona, Earth's auroral region, portions of Jupiter's inner magnetosphere, and comet atmospheres.

Existing plasma simulations generally fall into one of two categories, neither of which can treat semi-collisional plasmas satisfactorily: On the one hand one has simulation methods that treat the plasma as a fluid. (These include magnetohydrodynamics (MHD) and Hall-MHD simulations). Fluid-like simulations make the tacit assumption that the plasma is everywhere in local thermodynamic equilibrium. This amounts, in effect, to assuming very rapid collisions that wash out any interesting velocity-space features in the particles' distribution functions. As a consequence, all interesting kinetic features of the plasma beyond the lowest-order moments of the particle distribution functions are lost.

On the other hand one has fully kinetic simulations, including particle-in-cell (PIC) simulations and Vlasov simulations. PIC plasma simulations retain the kinetic features of the plasma, since the macro-particles sample the plasma distribution function in phase space, however they suffer from limited dynamical range and statistical noise due to having only a finite number of particles, and they generally ignore collisions. Vlasov simulations of the plasma provide low-noise modeling of the dynamics, yet they are computationally intensive (they must resolve a $2N$-dimensional phase space, where N is the number of spatial dimensions), and they generally do not include collisions.

Some PIC plasma simulations have been developed that can, in a limited way, model collisions. For example, early work by Shanny *et al.* (1967) demonstrated how one might add pitch-angle scattering to PIC simulations. Their algorithm did not treat the collisions self-consistently, however, which makes it applicable to a restricted subset of problems, such as electrons scattering off fixed ions. An alternative PIC collision model, called the "collision field" model has been developed by some of us (Jones *et al.*, 1996a,b, 1998). This model can treat collisions in a more self-consistent manner, however, like the collision model of Shanny *et al*, it requires prohibitively large numbers of particles to get high-fidelity results.

Ultimately we would like a computationally efficient and self-consistent way of including collisions in kinetic plasma simulations. Recent work by the authors has led to a method which we call "quiet Monte Carlo direct simulation" that has the potential to capture the physics of this challenging parameter regime. The presentation is structured as follows: First, we describe the theory underlying general particle methods and we discuss the advantages and shortcomings of Monte Carlo direct simulation. Then we describe an improvement

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which we call quiet Monte Carlo direct simulation (QMCDS) that has greatly reduced noise and and we show results of the application of this method to different systems, including diffusion and hydrodynamics. Finally, we discuss how the QMCDS method can be applied to kinetic simulation of plasmas. Preliminary results from this application of the method will be shown.

2 Theory Underlying Generalized Particle Methods

Suppose we are interested in finding a numerical solution of a partial differential equation (PDE) such as the Fokker Planck equation. This is generally a complicated problem and it can be time consuming on modern computing equipment. However, we note that the integration of ordinary differential equations (ODEs) is both straightforward (e.g. with Runge Kutta (Press *et al.*, 1992)) and efficient. The trick of particle methods is to exploit the relative ease of integrating ODEs by finding a way to represent a solution to the partial differential equation in terms of solutions of an equivalent set of ordinary differential equations. This is the essence of Monte Carlo methods, and it yields a powerful simplification to many problems.

One of the difficulties of Monte Carlo methods, however, is that, in general, a large number of particles are needed to sample the distribution function well. Consider the one-dimensional diffusion equation

$$\frac{\partial f}{\partial t} = D\frac{\partial^2 f}{\partial x^2}. \tag{1}$$

An equivalent formulation of the differential equation is in terms of a collection of random-walking particles, whose positions are given by the stochastic differential equation

$$x(t+dt) = x(t) + \sqrt{2D\,dt}\,N(0,1), \tag{2}$$

where $N(0,1)$ represents a random, normally distributed value with zero mean and unit variance. (See Gardiner (1994) for a discussion of how one obtains equivalent stochastic differential equations for a generalized Fokker Planck equation). The method of using particles to solve the diffusion equation, therefore, is straightforward: At time t one creates n particles at each point x_i on a spatial mesh where $f(x_i,t)$ is known, and each particle is made to carry a mass $f(x_i,t)/n$. Then, for each particle a realization is made of the random variable $N(0,1)$ using a random number generator, and this value is used in (2) to find the new position of the particle after a time $dt = \Delta t$ has elapsed. Finally, the particles are weighted back onto the mesh to find the updated mass function $f(x, t+\Delta t)$.

Though conceptually simple, this "Monte Carlo direct simulation" technique is very powerful. It requires no matrix inversions, which can be costly in higher dimensions, and all the operations require only local data, so the method would scale well on parallel computing architectures where communications latency is high. However, it has a disadvantage in that the updating formula (2) is statistical in nature—in

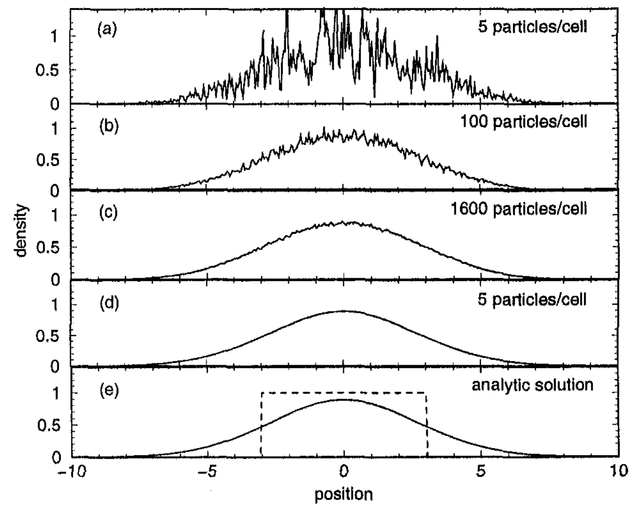

Fig. 1. Monte Carlo direct simulation of the diffusion of a slab. (The initial mass profile is shown in the dashed curve in panel (e) along with the analytic solution). Panels (a)–(c) are from a traditional Monte Carlo direct simulation; note how statistical noise in the solution is evident even with 1600 particles/cell. Panel (d) is a quiet Monte Carlo direct simulation of the same. The QMCDS simulation has essentially no statistical noise with 5 particles per cell. (100 simulation cells were used in this simulation).

order to get a good sampling of the random process one typically needs to go to large values of n, and even then the error associated with random sampling of $N(0,1)$ decreases slowly, scaling like $1/\sqrt{n}$. (See Fig. 1, panels (a)–(c)). Statistical errors associated with finite-particle effects lead to both noise and limited dynamical range in the simulation.

3 Quiet Monte Carlo Direct Simulation

We have found a remedy for the statistical difficulties associated with the random sampling of $N(0,1)$. Instead of giving every particle at a given point the same mass and drawing values at random from the distribution $N(0,1)$, we choose the set of masses m_j and corresponding N_j values ($j = 1\ldots n$) so that the same particle dynamics occur, but with the statistical error associated with having a finite number of particles minimized. In the case where the distribution $N(0,1)$ is normal, the natural choice is Gauss-Hermite weights and abscissas (Abramovitz and Stegun, 1972) for the m_i and N_i. With the simple replacement of $m_j \propto w_j$ and $N_j \propto a_j$, where w_j and a_j are the n-point Gauss-Hermite weights and abscissas, we find that very quiescent results may be obtained with only a few particles per cell.[1] (Compare Fig. 1 pan-

[1] A note of caution here: one must be careful of the weighting used to gather the particles onto the grid following the position update. E.g., the traditional linear weighting used in many PIC simulations is inherently diffusive, with a numerical diffusion coefficient that scales as $1/\sqrt{\Delta t}$, so the diffusion algorithm outlined above would not converge as $\Delta t \to 0$. To avoid this, a weighting method must be used that preserves the low-order moments of the mass dis-

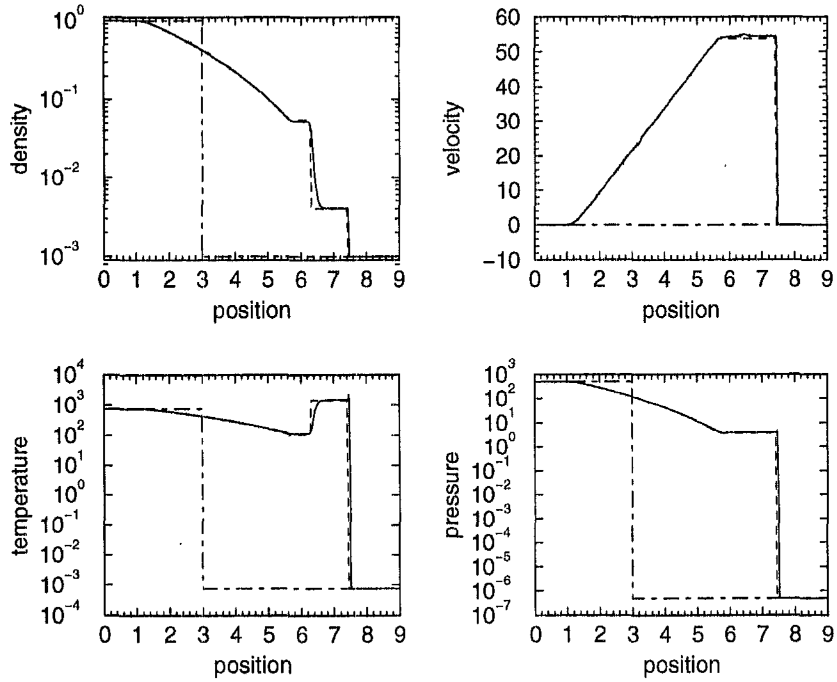

Fig. 2. Quiet Monte Carlo simulation results (solid curves) for a shock tube hydrodynamics test problem. The initial conditions (shown in the dot-dashed curve) have a density difference of 10^3 to 1 and an initial temperature difference of 10^6 to 1. The dashed curves are the exact solutions for the shock evolution. The simulation was run for a total of 246 time steps.

els (a)–(c) with panel (d)). Due to the quiet nature of the Gauss-Hermite sampling, we refer to this method as "quiet Monte Carlo direct simulation" (QMCDS). Note that in the QMCDS simulation method the particles are recreated anew every time step. Similar to the concept of "ephemeral particles" (Arter and Eastwood, 1995), this feature allows variations in the field quantities to be tracked over arbitrarily large dynamical ranges.

In summary, the QMCDS simulation does the following at every time step:

1. n new particles are generated in each cell via a "quiet start" from the moments accumulated onto the grid.

2. The particles are advanced.

3. Moments of quantities carried by the particles are accumulated back onto the grid, and the particles are destroyed.

In the case of simple diffusion, the "quiet start" of step 1 entails using the Gauss-Hermite weights and abscissas to construct the distribution of particles.

QMCDS is easily extensible to other systems, such as radiation transport (Lemons *et al.*, 2001) and Eulerian hydrodynamics (Jones *et al.*, 2000). For example, Pullin (1980) has performed Monte Carlo simulations of hydrodynamics by using the update formulae

$$x(t+dt) = x(t) + v\,dt \tag{3}$$

$$v(t+dt) = v(t) + \sqrt{2\sigma_v^2 dt}\,N(0,1), \tag{4}$$

tribution in each cell through the variance. Due to space limitations, we refer the interested to Jones *et al.* (2000) and Albright *et al.* (2001) where we have derived such a weighting.

where $\sigma_v^2(x(t),t)$ is the local value of the velocity variance, and he found that while his results were in general agreement with analytic predictions of the fluid behavior, the adverse level of statistical noise limited the applicability of his method. When we apply the QMCDS prescription for handling the random variable $N(0,1)$ to the Pullin's updating formulae, we find a quiescent, computationally efficient formulation of hydrodynamics. For illustration, in Fig. 2 we show QMCDS results of a particularly challenging hydrodynamics test problem, a one-dimensional shock tube with an initial jump in density of 10^3 to 1 across the interface, and a jump in temperature of 10^6 to 1. The QMCDS simulation is found to have both low-noise and large dynamical range. The simulation shown used 720 simulation cells and ten particles per cell (7200 total particles). The shock interface is tracked well, and with very little statistical noise.

4 Kinetic Simulation of Plasmas with QMCDS

The quiet Monte Carlo method works when one can replace the PDEs describing a system with equivalent Langevin equations. In the case of kinetic plasmas this means substituting the Vlasov equation with a Boltzmann collision operator (Lifshitz , 1981)

$$\frac{\partial f_i}{\partial t} + \boldsymbol{v}\cdot\nabla f_i + \frac{q}{m}\left(\boldsymbol{E} + \frac{\boldsymbol{v}\times\boldsymbol{B}}{c}\right)\cdot\frac{\partial f_i}{\partial \boldsymbol{v}} = \frac{1}{2}\frac{\partial}{\partial \boldsymbol{v}}\cdot\mathbf{D}\cdot\frac{\partial f_i}{\partial \boldsymbol{v}}, \tag{5}$$

with an equivalent set of (Itô) stochastic differential equations. Here $f_i(\boldsymbol{x},t)$ is the distribution function for species i, and the right hand side of (5) is the scattering operator. In the limit of weak scattering the stochastic differential equations have the form

$$\boldsymbol{x}(t+\Delta t) = \boldsymbol{x}(t) + \boldsymbol{v}(t)\,\Delta t \tag{6}$$

$$\boldsymbol{v}(t+\Delta t) = \boldsymbol{v}(t) + \frac{q}{m}\left(\boldsymbol{E} + \frac{1}{c}\boldsymbol{v}\times\boldsymbol{B} - \frac{1}{2}\frac{\partial}{\partial \boldsymbol{v}}\cdot\mathbf{D}\right)\Delta t + \sqrt{\mathbf{D}\,\Delta t}\cdot\boldsymbol{N}(0,1). \tag{7}$$

These equations, together with Maxwell's equations, give us a closed set of dynamical equations describing the evolution of the field quantities and the particles. The particles act as sources for the electric and magnetic fields, and the fields in turn allow the forces on the particles to be computed.

An attractive feature of the QMCDS simulation is that we can get high-accuracy, low-noise solutions to the underlying kinetic equations with only a modicum of particles. An intriguing possibility that we are currently examining is the application of the QMCDS method to the Vlasov-Maxwell equations, a simulation that would essentially be the quiet Monte Carlo analog of classical PIC simulations of plasmas. If successful, this would give us a simulation with the power and flexibility of traditional PIC simulations, but with fewer particles, greatly reduced noise, and arbitrary dynamical range.

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